





*Proposed*  
SCIENTIFIC CRITERIA DOCUMENT FOR THE DEVELOPMENT OF  
AN INTERIM PROVINCIAL WATER QUALITY OBJECTIVE  
FOR  
HEXACHLOROCYCLOPENTADIENE

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## PREFACE

The Ontario Ministry of Environment and Energy develops Provincial Water Quality Objectives for those substances deemed to be of greatest environmental concern in Ontario as determined through a screening process which considered persistence, potential to bioaccumulate, acute and chronic toxicity and potential presence in the aquatic environment. Alternatively, Ministry staff which have a direct responsibility for managing possible effects of these chemicals may request an evaluation.

Provincial Water Quality Objectives and Interim Provincial Water Quality Objectives (PWQO and Interim PWQO) are numeric or narrative criteria intended to protect all life stages of aquatic organisms for indefinite exposures and/or to protect recreational uses of water. PWQO for recreational uses, including swimming, are currently based on microbiological and aesthetic considerations. The potential for harmful effects from exposure to chemical substances during recreational uses will be considered when scientific information becomes available. Ontario Drinking Water Objectives and sport fish consumption guidelines are also considered in protection of human health. PWQO represent a desirable water quality for the protection of designated uses of surface waters in Ontario. Objectives do not take into account analytical detection or quantification limits, treatability or removal potential, socio-economic factors, natural background concentrations, or potential transport of contaminants among air, water and soil. These factors are considered in policies and procedures which govern the uses of PWQO, contained in the booklet, *Water Management: Policies, Guidelines and Provincial Water Quality Objectives of the Ministry of Environment and Energy* (1994), which deals with all aspects of Ontario's water management policy.

The process for deriving the PWQO and Interim PWQO is detailed in *Ontario's Water Quality Objective Development Process* (1992). The toxicology literature is reviewed for all of the following areas: aquatic toxicity, bioaccumulation, mutagenicity and aesthetic considerations. The final Objective is based on the lowest effect concentration reported for any of these factors on aquatic organisms as well as taste and odour considerations of the

water. Where there are reliable and adequate data, an Objective is developed using a safety factor. Where there are fewer data, an Interim PWQO is developed using an "uncertainty factor". The size of the uncertainty factor reflects the quality and quantity of data available and the potential of the material to bioaccumulate. Interim Objectives can be promoted to Objectives when sufficient reliable data become available.

PWQO are used to designate surface waters of the Province which should not be further degraded. They are also used in receiving water discharge assessments and may be included in Certificates of Approval which are issued to regulate effluent discharges. Where better water quality is required to protect other beneficial uses of the environment in a given location, appropriate criteria and factors, including public health considerations, are taken into account.



## SUMMARY

An Interim PWQO has been developed for hexachlorocyclopentadiene. The physical-chemical properties, aquatic toxicity, bioaccumulation potential, potential to damage genetic material, and taste and odour characteristics of hexachlorocyclopentadiene were considered in developing the Interim PWQO.

Hexachlorocyclopentadiene is a dense, pale-yellow or greenish-yellow, non-flammable liquid with a pungent odour. It is a chemical intermediate used in the production of organochlorine pesticides, fire retardant substances, dyes, pharmaceuticals, resins, and germicides (CCREM 1987). It was widely used as a precursor in the synthesis of the pesticides aldrin, chlordane, dieldrin, endrin, isodrin, heptachlor, endosulfan, chlordecone (Kepone), and dechlorane (mirex) (CCREM 1987). OMOE (1987) identified it as toxic and present in wastewater effluents in Ontario. Subsequent effluent monitoring in Ontario has revealed only minor releases of hexachlorocyclopentadiene to the aquatic environment.

The toxicity literature indicates that hexachlorocyclopentadiene is toxic to aquatic life. The available chronic studies report a 30-d LC50 for hexachlorocyclopentadiene of 0.0067 mg/L for fathead minnow and a 21-d LOEC of 0.019 mg/L for *Daphnia magna*. Reported 96-h LC50s for fish range from 0.007 to 0.18 mg/L. Acute LC50s for aquatic invertebrates range from 0.039 mg/L for *Daphnia magna* to 2.3 mg/L for mosquito larvae. Hexachlorocyclopentadiene does not appear to be persistent in the water column. It probably is rapidly removed from water, mainly by photolysis and possibly volatilization in shallow waters and by hydrolysis and biodegradation in deeper waters. Accumulation in aquatic biota may be a concern based on chemical and physical properties, but data on bioaccumulation do not support this conclusion. Accumulation in sediments may be of concern. Available monitoring studies suggest only minor contamination of the aquatic environment as a result of this chemical.

An Interim Provincial Water Quality Objective<sup>1</sup> is derived herein for hexachlorocyclopentadiene, as there were insufficient data to develop a Provincial Water

Quality Objective. The recommended Interim Provincial Water Quality Objective was calculated by dividing a 30-day LC50 of 0.0067 mg/L for fathead minnow by a final uncertainty factor of 105 to give an interim objective of 0.00006 mg/L or 0.06 µg/L.

This Interim Provincial Water Quality Objective should be protective of aquatic life during indefinite exposures to hexachlorocyclopentadiene in water. It should also protect against odour and possibly taste impacts in water.

<sup>1</sup> This process is described in *Ontario's Water Quality Objective Development Process* (OMOE 1992a).

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## 1.0 INTRODUCTION

This document describes the development of an Interim Provincial Water Quality Objective (Interim PWQO) for hexachlorocyclopentadiene. This chemical was identified by the Effluent Monitoring Priority Pollutants List (OMOE 1987) as toxic and present in effluents discharged to Ontario surface waters. Subsequent effluent monitoring in Ontario has revealed only minor releases of hexachlorocyclopentadiene to the aquatic environment.

Hexachlorocyclopentadiene is a dense, pale-yellow or greenish-yellow, non-flammable liquid with a pungent odour (WHO 1991).

Alternate names include:

perchlorocyclopentadiene, 1,2,3,4,5,5-hexachloro-1,3-cyclopentadiene, hexachloro-1,3-cyclopentadiene, HEX, and C-56.

Literature cited in the preparation of this Interim PWQO is current to December 1994.

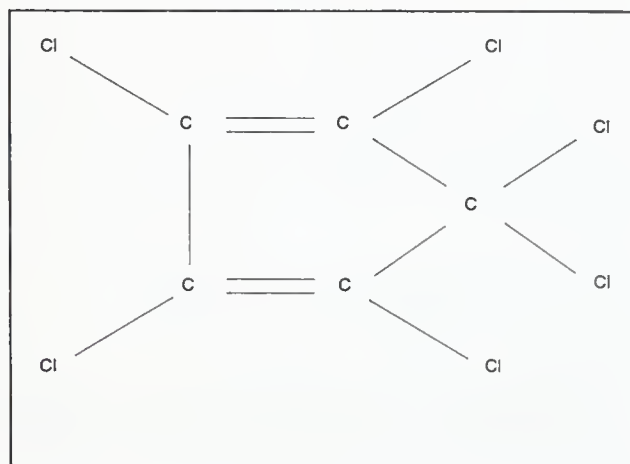


Figure 1 - hexachlorocyclopentadiene

## 1.1 PRODUCTION AND USES

Hexachlorocyclopentadiene is a chemical intermediate used in the production of organochlorine pesticides, fire retardant substances, dyes, pharmaceuticals, resins, and germicides (CCREM 1987). It was widely used as a precursor in the synthesis of the pesticides aldrin, chlordane, dieldrin, endrin, isodrin, heptachlor, endosulfan, chlordecone (Kepone), and dechlorane (mirex) (CCREM 1987). While restrictions on many of the pesticides produced from hexachlorocyclopentadiene have decreased its use as a chemical intermediate, its use in the manufacturing of flame retardants has increased (U.S. EPA 1980).

No production or use information was found for Canada, but in 1988, world production was approximately 15,000 tonnes (WHO 1991). The total production in the United States between 1962 and 1975 was estimated at 300 million kilograms (NRC 1978).

Hexachlorocyclopentadiene may enter the aquatic environment through industrial discharges from facilities which manufacture or use this compound as a chemical intermediate. It may also have entered the environment during pesticide use if present as an impurity in pesticides produced from hexachlorocyclopentadiene. For example, at one time it comprised as much as one percent of commercial chlordane (U.S. EPA 1980).

While no Ontario airborne release information was found, the U.S. EPA's 1987 Toxic Release Inventory reported that more than 500 kg of hexachlorocyclopentadiene was released from the Occidental Chemical Corporation site at Niagara Falls, New York. Most of this release was to the air.

## 1.2 PROPERTIES AND FATE

A summary of the physical-chemical properties is given in Table 1 in the appendices.

Most reported water solubilities for hexachlorocyclopentadiene range between 0.8 to 1.8 mg/L, (e.g. U.S. EPA 1980, WHO 1991, Callahan *et al.* 1979, Wolfe *et al.* 1982).

As it is highly photoreactive, photolysis is expected to be a primary removal mechanism in aquatic systems (Callahan *et al.* 1979, CCREM 1987). By exposing test vessels to actual sunlight, and using both distilled and natural river water, Wolfe *et al.* (1982) measured photolytic half-lives of less than 10 minutes. Chou *et al.* (1987) measured photolytic half-lives of less than four minutes. Results were obtained by exposing samples using tap water, distilled water, and creek water to sunlight. The primary degradation products were found to be 2,3,4,4,5-pentachloro-2-cyclopentenone, hexachloro-2-cyclopentenone and hexachloro-3-cyclopentenone.



Hydrolysis of hexachlorocyclopentadiene may also be significant fate process. Zepp *et al.* (1979) determined a hydrolytic half-life of approximately 14 days at 25 °C. This reaction was found to be independent of pH, but dependant on temperature. Wolfe *et al.* (1982) and Yu and Atallah (1977) measured the hydrolytic half-life as 3-11 days at 25-30 °C and pH of 5-9. Another study by Chou and Griffin (1983) which carefully prevented evaporation and photochemical reactions, found a hydrolytic half life of approximately three months. Hydrolysis, along with biodegradation, may be the most significant degradation process in deep, non-flowing waters (WHO 1991).

Based on model simulations of several types of aquatic ecosystems, volatilization was determined to be a significant removal process in turbid rivers but less significant in lakes and ponds (Zepp *et al.* 1979, Wolfe *et al.* 1982). Laboratory tests using <sup>14</sup>C-labelled hexachlorocyclopentadiene seem to confirm that volatilization will be greater in moving waters (Kilzer *et al.* 1979). An estimated total loss of approximately 18-24% would be expected over a 24-hour period if static conditions were maintained.

Callahan *et al.* (1979) suggest that biodegradation does not appear to be an important removal mechanism in the aquatic environment, however, WHO (1991) suggests that it may be a key mechanism in deeper water where some other degradation processes are precluded. Howard *et al.* (1991) estimate aqueous biodegradation of between one to four weeks under aerobic conditions and four to 16 weeks under anaerobic conditions. Lu *et al.* (1975) reported that metabolism of hexachlorocyclopentadiene by algae, snails, mosquito larvae, and fish following a 33-d exposure was minor. In this study, some of the breakdown products included hexachloro-2-cyclopentenone and hexachloro-3-cyclopentenone.

Reported log octanol/water partition coefficients for hexachlorocyclopentadiene range between 3.99 and 5.51 (Zepp *et al.* 1979; Veith *et al.* 1979; Wolfe *et al.* 1982, Leo and Weininger 1988). Mackay (1982), however, questioned the validity of the high value of 5.51 reported by Veith *et al.* (1979). These log octanol/water partition coefficients suggest that sorption to particulate matter and bioaccumulation may occur. Some limited sediment monitoring data

support the conclusion that hexachlorocyclopentadiene accumulates in sediments and that it may persist in the sediment even after a discharge discontinues (WHO 1991). Based on the results of a fate and transport model, however, Zepp *et al.* 1979 suggest that sorption to sediments is not as important as other competing fate processes. Bioaccumulation is discussed in greater detail in Section 3.0.

The following table summarizes the predicted fate of hexachlorocyclopentadiene in four different ecosystems:

Summary of Results of A Computer Simulation of the Fate and Transport of Hexachlorocyclopentadiene in Four Typical Aquatic Environments<sup>a</sup>

	River	Pond	Eutrophic Lake	Oligotrophic Lake
Distribution (percent)				
Water Column	1.22	14	12.97	2.91 <sup>b</sup>
Sediment	98.78	86	87.03	97.09
Recovery time <sup>c</sup> (days)	52	81	58	87
Load reduction (percent) by processes:				
Hydrolysis	8.04	17.85	8.29	16.50
Oxidation	0.00	0.00	0.00	0.00
Photolysis	18.68	80.39	89.18	82.41
Biodegradation (biolysis)	0.57	0.23	0.30	0.01
Volatilization	0.69	1.33	1.56	1.08
Export <sup>d</sup>	72.02	0.20	0.01	0.00

<sup>a</sup> Adapted from Wolfe *et al.* (1982), with correction applied.

<sup>b</sup> Value was incorrectly reported as 32.91 in original paper.

<sup>c</sup> The time needed to reduce steady-state concentration by five half-lives.

<sup>d</sup> Physical loss from the system by any pathway other than volatilization.

Lu *et al.* (1975) present measured values showing the aquatic fate of <sup>14</sup>C-labelled hexachlorocyclopentadiene in a model aquatic ecosystem. After 33 days it was stored as 33%



of extractable  $^{14}\text{C}$  in alga, 50% in snails, 46% in mosquito larvae, and 41% in fish, demonstrating considerable environmental stability.

Several monitoring studies have analyzed for hexachlorocyclopentadiene. Environment Canada found no detectable concentration in 13 effluent samples from an industrial plant at Cornwall, Ontario (Environment Canada 1984). As part of the Ontario Ministry of Environment and Energy's Municipal Industrial Strategy for Abatement (MISA), hexachlorocyclopentadiene was monitored for in the effluents of the Pulp and Paper Sector, the Organic Chemical Manufacturing Sector, and in a study of sewage treatment plants. Based on this monitoring, potential dischargers of hexachlorocyclopentadiene can be found near Fort Frances, Thorold, Cornwall, and Sarnia, Ontario. The results are summarized below:

MISA Sector	Hexachlorocyclopentadiene Monitoring Results
Pulp and Paper (OMOE 1991)	<ul style="list-style-type: none"> <li>detected in 30% of effluent samples from the sulphate (kraft) subcategory (9 different plants); the average concentration was 0.02 <math>\mu\text{g/L}</math> and the maximum was 0.34 <math>\mu\text{g/L}</math>.</li> <li>detected in 11% of effluent samples from the sulphite-mechanical subcategory (8 different plants); the average concentration was below detection and the maximum concentration reported was 0.05 <math>\mu\text{g/L}</math>.</li> <li>detected in 16% of effluent samples from the deinking-board-fine tissue subcategory (8 different plants); the average concentration was 0.03 <math>\mu\text{g/L}</math> and the maximum concentration reported was 0.41 <math>\mu\text{g/L}</math>.</li> </ul>
Organic Chemical Manufacturing (OMOEE 1993 - unpublished)	<ul style="list-style-type: none"> <li>found in the effluent of 2/20 plants in the sector.</li> <li>at Cornwall Chemicals Ltd., Cornwall, the 12 month average concentration value was 0.013 <math>\mu\text{g/L}</math> and the loading was less than one gram/day.</li> <li>at Dow Chemical Canada Inc., Sarnia, the 12-month average effluent concentrations at eight sampling points ranged between 0.0017 and 0.166 <math>\mu\text{g/L}</math>. These sampling points either discharged to the river or to a sewer leading to the river; the loadings from any of four outfalls were each less than one gram/day, while one outfall discharged 3 grams/day.</li> </ul>
Municipal WPC Plants (OMOE 1988)	<ul style="list-style-type: none"> <li>detected in 5 of 276 raw sewage samples and in no other effluents streams.</li> </ul>

The MISA Regulation Method Detection Limit (RMDL) for hexachlorocyclopentadiene in water was 0.01 µg/L. For all but one of the Dow Chemical Canada Inc., Sarnia sampling points, the average concentration did not qualify as "found" as the concentration was below the MISA RMDL. However, these "below RMDL" data are still reported (OMOEE 1993). There are no other data on ambient concentrations of hexachlorocyclopentadiene in Ontario waters.

A review of the concentrations of priority pollutants in both industrial effluents and ambient surface waters in the United States indicated that the median concentration of hexachlorocyclopentadiene was less than 10 µg/L in both media (Staples *et al.* 1985).

The Ontario MOEE's Drinking Water Surveillance Program occasionally finds trace concentrations of hexachlorocyclopentadiene in treated drinking water, while seldom detecting any in the intake water. It appears to be formed during the chlorination process, but levels (maximum concentration found was 0.6 µg/L) are below the suggested safe levels for drinking water (H. Graham, pers. comm., 1993). Meirer *et al.* (1985) demonstrated that hexachlorocyclopentadiene can be formed by the chlorination of water containing humic acid.

In summary, hexachlorocyclopentadiene does not appear to be persistent in the water column. It is probably rapidly removed from water, mainly by photolysis and possibly volatilization in shallow waters and by hydrolysis and biodegradation in deeper waters. Accumulation in aquatic biota may be a concern based on chemical and physical properties, but data on bioaccumulation do not support this conclusion (see Section 3.0). Accumulation in sediments may be of concern. Available monitoring studies suggest only minor contamination of the aquatic environment as a result of this chemical.

## 2.0 TOXICITY TO AQUATIC ORGANISMS

Criteria used for classifying the quality of available toxicity data as either primary or secondary information are described in the document titled *Ontario's Provincial Water*

*Quality Objective Development Process* (OMOE 1992a). In general, primary toxicity studies have acceptable test procedures, conditions, and controls, measured toxicant concentrations, and flow-through or renewal conditions. Secondary toxicity studies usually have unmeasured toxicant concentrations, static bioassay conditions, and unsatisfactory reporting of experimental data. Generally, acute toxicity studies are those having a test duration of less than or equal to 96 hours for vertebrates or less than or equal to 48 hours for invertebrates. Chronic studies include complete life cycle tests or partial life cycle tests involving early life stages.

All toxicity data are summarized in Table 2.

## 2.1 ACUTE TOXICITY

This section addresses the acute toxicity of hexachlorocyclopentadiene. (NOTE: The acute toxicity studies by Spehar *et al.* (1979) were considered primary data, while the results of all other acute studies were classified as secondary data or tertiary data. See Table 2.)

### 2.1.1 Vertebrates

Spehar *et al.* (1979) determined the toxicity of hexachlorocyclopentadiene to larval and early juvenile fathead minnows (*Pimephales promelas*). The 96-h LC50 was 0.0070 mg/L. Test concentrations were measured, a flow-through system was used, appropriate controls were maintained and water chemistry was provided. This same study was also described (in greater detail) in U.S. EPA (1977). A study using a static test and 30-d old fathead minnows was also conducted in the same laboratory (Geiger 1987, unpublished data). A 96-h EC50 of 0.030 mg/L was estimated. The effects noted were loss of schooling behaviour, swimming near the tank bottom, hyperactivity, over-activity to stimuli, increased respiration, and bright red gills. However, these results have been considered as secondary information as the test concentrations were highly variable and the solutions were not renewed. Controls were maintained and water chemistry was provided in this study.

Henderson (1956) exposed fathead minnows to hexachlorocyclopentadiene in soft (40 mg/L  $\text{CaCO}_3$ ) and hard (400 mg/L  $\text{CaCO}_3$ ) water. The 96-h LC50s were 0.104 mg/L in soft water and 0.078 mg/L in hard water, suggesting little effect of hardness on acute toxicity. The test was conducted under static conditions and water concentrations were not measured.

Henderson (1956) also evaluated the effect of the method used to add the hexachlorocyclopentadiene to the dilution water. Two methods of addition were tested using hard water (400 mg/L  $\text{CaCO}_3$ ). A 0.01% acetone solution and a 0.001% suspension of an emulsion prepared in a blender were compared. The corresponding 96-h LC50 using acetone was 0.078 mg/L, as noted above. The 96-h LC50 using the 0.001% suspension was 0.059 mg/L. The authors concluded that there was little difference between the two methods of addition on the toxicity. The tests were conducted under static conditions and toxicant concentrations were not measured. Partial water chemistry was reported.

Buccafusco and LeBlanc (1977) studied the acute toxicity of hexachlorocyclopentadiene to fathead minnows, bluegill sunfish and channel catfish (*Ictalurus punctatus*). The corresponding 96-h LC50s were 0.180 mg/L, 0.130 mg/L and 0.097 mg/L, respectively. The 48-h LC50s were 0.210 mg/L, 0.150 mg/L and 0.150 mg/L, respectively, and the 24-h LC50s were 0.240 mg/L, 0.170 mg/L and 0.190 mg/L, respectively. Corresponding NOECs of 0.087, 0.065 and 0.056 mg/L were also reported. The tests were conducted under static conditions and water concentrations were not measured. Partial water chemistry was provided.

Davis and Hardcastle (1959) reported the acute toxicity of hexachlorocyclopentadiene to fingerling bluegill sunfish (*Lepomis macrochirus*) and largemouth bass (*Micropterus salmoides*). The 24-, 48-, and 96-h LC50s for bluegill sunfish were >500, 30, and 25 mg/L, respectively. The corresponding LC50s for largemouth bass exposed to hexachlorocyclopentadiene were >500, 35, and 20 mg/L, respectively. Testing was conducted under static conditions, the nominal toxicant concentrations exceeded the solubility of hexachlorocyclopentadiene, and toxicant concentrations were not measured. The test water was collected from the field and partial water chemistry was provided.



Sinhaseni *et al.* (1983) reported that a concentration of 0.13 mg/L was lethal to rainbow trout (*Oncorhynchus mykiss*) within 6.5 hours of exposure. A flow-through exposure system was used, however, test concentrations were not measured in the exposure vessels. No information on water chemistry was provided and a small sample size was used (5 fish). Exposure to hexachlorocyclopentadiene resulted in an initial 1.86 times increase in oxygen consumption. The authors suggested that a mechanism of toxic action for hexachlorocyclopentadiene may be increased oxygen consumption combined with impaired oxidative ATP synthesis.

The average time to death for sea lamprey (*Petromyzon marinus*) larvae exposed to 5.0 mg/L of hexachlorocyclopentadiene was 11 and 1 hours for two replicate tests, and at 1 mg/L time to death was 30 minutes, on average (Applegate *et al.* 1957). No explanation was given for why the sea lamprey appeared to be more sensitive at 1.0 mg/L than 5.0 mg/L. Rainbow trout exposed to 5.0 mg/L were killed after 15 and 30 minutes in two replicate tests, and at 1.0 mg/L time to death was 1 hour, on average. The average times to death for bluegill sunfish exposed to 5.0 mg/L of hexachlorocyclopentadiene were 15 and 30 minutes for two replicate tests, and at 1.0 mg/L time to death was 30 minutes. No effect was observed over 24 hours at 0.1 mg/L for all three species. All tests were conducted under static conditions and water concentrations were not measured. Partial water chemistry was provided.

Mortality resulted when northern squawfish (*Ptychocheilus oregonensis*), chinook salmon (*Oncorhynchus tshawytscha*), and coho salmon (*Oncorhynchus kisutch*) were exposed to 10 mg/L of hexachlorocyclopentadiene for 3 hours (MacPhee and Ruelle 1969). One fish of each species was tested in the same 4 L chamber. The test was conducted under static conditions and water concentrations were not measured. As well, the exposure concentration exceeded the solubility of hexachlorocyclopentadiene. Partial water chemistry was provided.

Podowski *et al.* (1991) reported LT50s (median lethal times) ranging from 9.1 to 16.6 hours for goldfish (*Carassius auratus*) at a hexachlorocyclopentadiene concentration of 0.18 mg/L.

The tests were conducted under static conditions and water concentrations were not measured. No other information on test conditions and procedures were provided.

### 2.1.2 Invertebrates

Kuhn *et al.* (1989) reported a 24-h EC50 (effect not specified) of 0.21 mg/L for hexachlorocyclopentadiene using 24 hour-old *Daphnia magna*. The test was conducted under static conditions and toxicant concentrations were not measured. Partial water chemistry was provided.

Buccafusco and LeBlanc (1977) reported 48-h and 24-h LC50s of 0.039 and 0.13 mg/L, respectively, for *Daphnia magna*. A NOEC of 0.018 mg/L was also reported. Testing was conducted under static conditions, and water concentrations were not measured. Partial water chemistry was provided.

Both 48-h and 24-h LC50s for *Daphnia magna* were reported by Vilkas (1977). The LC50s were 0.052 and 0.093 mg/L, respectively. A NOEC of 0.032 mg/L was also reported. The tests were conducted under static conditions, water concentrations were not measured, and only partial water chemistry was provided.

Lu *et al.* (1975) reported an LC50 of 2.3 mg/L for hexachlorocyclopentadiene using mosquito larvae (*Culex*). No information on exposure duration, test conditions, and procedures were given. The test is assumed to be of acute duration. It has been classified as tertiary information and has not been used for setting an Interim PWQO.

## 2.2 CHRONIC TOXICITY

This section addresses the chronic toxicity of hexachlorocyclopentadiene. (NOTE: The chronic toxicity studies by Spehar *et al.* (1979) and Kuhn *et al.* (1989) were considered

primary data, while the results of all other chronic studies were classified as secondary or tertiary data.)

#### 2.2.1 Vertebrates

Spehar *et al.* (1979) determined the toxicity of hexachlorocyclopentadiene to larval and early juvenile fathead minnows over a 30 day period. The 30-day LC50 was 0.0067 mg/L. This value is very similar to the 96-h LC50 (0.0070 mg/L) described earlier, suggesting that a median lethal threshold was attained within 4 days. Test concentrations were measured, a flow-through system was used, appropriate controls were maintained, and water chemistry was provided. The highest concentration tested at which there was no significant effect, compared to controls, on survival, length, or weight of juvenile fathead minnows (i.e. the NOEC) over the 30 day exposure was 0.0037 mg/L.

#### 2.2.2 Invertebrates

Kuhn *et al.* (1989) reports a 21-d NOEC of 0.009 mg/L for hexachlorocyclopentadiene using 24 hour-old *Daphnia magna*. From the description of the test procedures, the 21-d LOEC can be determined. The 21-d LOEC (parent animal mortality) was 0.019 mg/L. The testing was conducted under renewal conditions to maintain the water concentration of hexachlorocyclopentadiene (renewed 3-times weekly). Toxicant concentrations were measured during the test. Partial water chemistry was provided.

#### 2.2.3 Other Organisms (Algae, Bacteria, Protozoa)

Using the algae *Scenedesmus subspicatus*, Kuhn and Pattard (1990) studied the effect of hexachlorocyclopentadiene on biomass and growth. The 48-h IC50s (median inhibition concentrations) for biomass and growth were 0.08 and 0.24 mg/L, respectively. The studies were conducted under static conditions and water concentrations were not measured. Partial water chemistry was reported.

## 2.3 SUMMARY OF TOXICITY DATA

The toxicity data for hexachlorocyclopentadiene is summarized in Table 2 and in Figure 2. A wide range of LC50s are presented for hexachlorocyclopentadiene. The available chronic studies report a 30-d LC50 for hexachlorocyclopentadiene of 0.0067 mg/L for fathead minnow and a 21-d LOEC of 0.019 mg/L for *Daphnia magna*. Reported 96-h LC50s for fish range from 0.007 to 0.18 mg/L. Acute LC50s for aquatic invertebrates range from 0.039 mg/L for *Daphnia magna* to 2.3 mg/L for mosquito larvae. Noteworthy is the increased toxicity of hexachlorocyclopentadiene that is measured when flow-through or renewal exposure systems are used, highlighting the unstable nature of hexachlorocyclopentadiene in water.

## 3.0 BIOACCUMULATION

Spehar *et al.* (1979) determined the bioconcentration of hexachlorocyclopentadiene using one-day-old fathead minnow larvae over a 30-day exposure period with flow-through exposure conditions. Five concentrations of hexachlorocyclopentadiene ranging from 0.00078-0.0091 mg/L and a control sample were tested. Test concentrations were measured daily in the exposure vessel. Residue analyses were conducted on whole-fish on a wet-weight basis. Residues of hexachlorocyclopentadiene in fathead minnows after 30 days exposure were less than 0.0001 mg/g at all concentrations tested. A bioconcentration factor of less than 11 was determined.

The bioconcentration factor for adult fathead minnows (approximately 6 months old) exposed to 0.0209 mg/L hexachlorocyclopentadiene under flow-through conditions for 32 days was 29 (Veith *et al.* 1979). Hexachlorocyclopentadiene concentrations were measured in the exposure vessel on every weekday. Concentrations in the fish were analyzed on a whole-fish basis.



Oliver and Niimi (1985) exposed 200 g rainbow trout to 7 ng/L hexachlorocyclopentadiene for 96 days under measured, flow-through exposure conditions. Hexachlorocyclopentadiene was not detected in fish after the 96-day exposure, suggesting no bioconcentration of the chemical. The analytical detection limit was not reported, however.

Podowski and Khan (1984) determined the bioconcentration of  $^{14}\text{C}$ -labelled hexachlorocyclopentadiene in 0.5-1.7 g goldfish using a static with renewal exposure system. In one experiment, the bioconcentration factor, based on radioactivity, in goldfish exposed to 0.004 mg/L hexachlorocyclopentadiene peaked at 1297 after 8 days, then decreased to 1148 after 16 days. In a second experiment, the bioconcentration factor in goldfish exposed in a static without renewal exposure system peaked at 323 after 2 days, then decreased to 100 after 16 days. Hexachlorocyclopentadiene concentrations in fish and water were based on total radioactivity with no differentiation between parent compound and metabolites. Thus, the bioconcentration factors represent both the parent compound and possible metabolites.

Bioconcentration of  $^{14}\text{C}$  hexachlorocyclopentadiene in algae (*Chlorella fusca* var. *vacuolate*) and in golden orfe (*Leuciscus idus melanotus*) was studied by Freitag *et al.* (1982). The *Chlorella* were exposed to 0.050 mg/L hexachlorocyclopentadiene in a stoppered Erlenmeyer flask for 24 h at 20-25 °C. After 24 hours, 31 percent of the applied radioactivity was found in the algae. This corresponded to a bioconcentration factor of 1090 (based on wet weight). These data are also presented by Geyer *et al.* (1981). Golden orfe (1.5 g) were exposed to a median concentration of 0.048 mg/L  $^{14}\text{C}$  labelled hexachlorocyclopentadiene for three days at 20-25 °C. The exposure was static with daily renewal of the solution. After 3 days, the bioconcentration factor was 1230 (based on whole-fish, wet weight).

$^{14}\text{C}$  labelled hexachlorocyclopentadiene was applied to terrestrial plants in a 33-day laboratory model ecosystem study (Lu *et al.* 1975). Caterpillar larvae consumed these plants. Hexachlorocyclopentadiene reached the water as caterpillar faeces, plant matter and as the larvae themselves contaminated the underlying moist sand, permitting distribution of hexachlorocyclopentadiene by the water throughout the model ecosystem. A peak

concentration of 0.031 mg/L was reached in the water after 14 days, and decreased to 0.016 mg/L after 33 days. Percentages of total extractable  $^{14}\text{C}$  hexachlorocyclopentadiene within each organism were reported. The percentages of total extractable  $^{14}\text{C}$  recovered as unmetabolized hexachlorocyclopentadiene in each of the organisms were as follows: 33 percent was unmetabolized hexachlorocyclopentadiene in alga (*Oedogonium cardiacum*), 50 percent in snails (*Physa* sp.), 46 percent in mosquito larvae (*Culex pipiens quinquefasciatus*), and 41 percent in fish (*Gambusia affinis*). The corresponding bioaccumulation factors were 341 for alga, 1634 for snails, 929 for mosquito larvae and 448 for fish. Only two percent of total extractable  $^{14}\text{C}$  in the water was recovered as unmetabolized hexachlorocyclopentadiene. These values may underestimate the extent of metabolism, since acetone extractable polar compounds were not considered in the calculations (WHO, 1991 and U.S. EPA, 1984).

Based on its lipophilicity, hexachlorocyclopentadiene would be expected to bioaccumulate. Log octanol/water partition coefficients of between 3.99 and 5.51 suggest that bioaccumulation may occur. As well, bioconcentration factors of greater than 1,000 were reported in studies using  $^{14}\text{C}$ -labelled hexachlorocyclopentadiene. These studies suggest that hexachlorocyclopentadiene may bioaccumulate, however, caution is required in the interpretation of studies using  $^{14}\text{C}$ -labelled compounds because of the need to differentiate between the parent compound and metabolites. The bioaccumulation factors derived from a short-term model ecosystem study suggest a moderate accumulation potential (Lu *et al.* 1975). However, in the same study the compound did not biomagnify between trophic levels. Steady-state, measured, flow-through bioconcentration factors of 11 and 29 were reported by Spehar *et al.* (1979) and Veith *et al.* (1979), respectively. This suggests that hexachlorocyclopentadiene does not bioaccumulate. Similarly, Oliver and Niimi (1985) found no bioconcentration of hexachlorocyclopentadiene. Podowski and Khan (1984) demonstrated that gold fish were able to metabolize and excrete hexachlorocyclopentadiene. For the purpose of setting an Interim PWQO, the weight of evidence suggests that hexachlorocyclopentadiene is not bioaccumulative (see Section 6.0). WHO (1991) and U.S. EPA (1984) have also concluded that hexachlorocyclopentadiene does not bioaccumulate significantly.

#### **4.0      IMPACTS ON TASTE AND ODOUR OF WATER AND FISH TISSUES**

An odour threshold concentration for hexachlorocyclopentadiene in water of 0.001 mg/L was reported by Zoeteman *et al.* (1974) and WDNR (1989). U.S. EPA (1980) cites a study by Naishstein and Lisovskaya (1965) which determined the lowest concentration of hexachlorocyclopentadiene capable of altering the smell and taste of water. The study reported that the lower confidence limit of the mean threshold response concentration was 1.4 µg/L for odour and 1.6 µg/L for taste.

No information was found indicating that hexachlorocyclopentadiene taints fish tissues.

#### **5.0      OTHER EFFECTS**

##### **5.1      MUTAGENICITY**

In its health assessment document for hexachlorocyclopentadiene, U.S. EPA (1980) reviewed the mutagenicity of hexachlorocyclopentadiene. All the literature reviewed indicated that it was non-mutagenic. WHO (1991) reviewed a number of non-aquatic studies on the mutagenicity of hexachlorocyclopentadiene. None of the studies reported mutagenic activity associated with hexachlorocyclopentadiene. Since there are no mutagenicity studies on freshwater organisms available, a numeric objective to protect against such effects could not be derived.

##### **5.2      DERMAL EXPOSURE**

No studies were found which report effects from dermal exposure to waterborne hexachlorocyclopentadiene. WHO (1991) notes that there are studies which report discolouration of the skin, and in some cases toxic responses resulting from a dermal application of pure, undiluted hexachlorocyclopentadiene to human skin.

## 6.0 DERIVATION OF THE INTERIM WATER QUALITY OBJECTIVE

There are insufficient toxicological data to develop a Provincial Water Quality Objective for hexachlorocyclopentadiene. Therefore, following standard procedures an Interim Objective is calculated using the available toxicological information (OMOE 1992a). These calculations are described in this section.

Where interim objectives are set to protect aquatic life, the interim objective is derived by dividing the lowest adverse effect concentration by an "uncertainty factor". The size of the uncertainty factor reflects the quality and quantity of data available and the potential of the material to bioaccumulate.

Limits for chemicals in waters used for recreation (i.e. human exposure through dermal adsorption and accidental ingestion) have not been recommended by the Federal-Provincial Working Group on recreational water quality because of insufficient scientific information (Health and Welfare Canada 1992). Therefore, a recreational use water quality guideline for the protection of human health is not recommended at this time.

While dermal effects resulting from exposure of human skin to pure hexachlorocyclopentadiene have been reported (see Section 5.0), it is unlikely that recreational water users in Ontario will encounter concentrations in surface waters that would represent a threat. Available studies suggest that hexachlorocyclopentadiene is only present at very low concentrations or is not detectable in Ontario surface waters.

### 6.1 CALCULATION OF FINAL UNCERTAINTY FACTOR

The choice of a baseline uncertainty factor depends on the BCF of hexachlorocyclopentadiene. Bioconcentration factors of 11 and 29 were reported by Spehar *et al.* (1979) and Veith *et al.* (1979), respectively. As these BCFs are less than 1000, the baseline uncertainty factor used is 1000 (OMOE 1992a). (See Table 3.)

The final uncertainty factor was calculated using the following studies:

#### 6.1.1 Acute Toxicity Studies

1. Spehar *et al.* (1979) determined the toxicity of hexachlorocyclopentadiene to larval and early juvenile fathead minnows. The 96-h LC50 was 0.0070 mg/L. Test concentrations were measured, a flow-through system was used, appropriate controls were maintained, and water chemistry was reported. This study is classified as primary acute toxicity information for a warm-water fish species.
2. Buccafusco and LeBlanc (1977) reported the acute toxicity of hexachlorocyclopentadiene to channel catfish. The 96-h LC50 was 0.097 mg/L. The test was conducted under static conditions and water concentrations were not measured. Only partial water chemistry was reported. This study is classified as secondary acute toxicity information for a warm-water fish species.
3. Sinhaseni *et al.* (1983) reported that a concentration of 0.13 mg/L of hexachlorocyclopentadiene caused 100 percent mortality to rainbow trout within 6.5 hours of exposure. A flow-through system of exposure was used, however, test concentrations were not measured in the exposure vessels. No information on water chemistry was provided and only five fish were tested. This study is classified as secondary acute toxicity information for a cold-water fish species.
4. Kuhn *et al.* (1989) reports a 24-h EC50 of 0.21 mg/L for hexachlorocyclopentadiene using 24 hour-old *Daphnia magna*. The test was conducted under static conditions and toxicant concentrations were not measured. Partial water chemistry was reported. This study is classified as secondary acute toxicity information for an invertebrate.



### 6.1.2 Chronic Toxicity Studies

1. Spehar *et al.* (1979) determined the toxicity of hexachlorocyclopentadiene to larval and early juvenile fathead minnows over a 30 day period. The 30-day LC50 was 0.0067 mg/L. Test concentrations were measured, a flow-through system was used, appropriate controls were maintained, and water chemistry was reported. This study has been classified as primary chronic toxicity information for a warm-water fish species. This was the lowest measured effect concentration in the literature.
2. An acute-chronic ratio of 1.3 (0.0070/0.0067) was derived in the study by Spehar *et al.* (1979). This ratio was applied to the acute 96-h LC50 of 0.130 mg/L for bluegill sunfish (Buccafusco and LeBlanc 1977) to estimate a chronic toxicity value. The calculation predicts a 30-d LC50 chronic toxicity value of 0.124 mg/L for bluegill sunfish. The study by Buccafusco and LeBlanc (1977) was conducted under static conditions and water concentrations were not measured. The chronic toxicity endpoint simulated by this calculation is used on Table 2 to reduce the final uncertainty factor.
3. Kuhn *et al.* (1989) reports a 21-d LOEC (parent animal mortality) of 0.019 mg/L for hexachlorocyclopentadiene using 24 hour-old *Daphnia magna*. The testing was conducted under renewal conditions and toxicant concentrations were measured in the exposure vessels. Partial water chemistry was reported. This study has been classified as primary chronic toxicity information for an invertebrate.
4. Kuhn and Pattard (1990) reported a 48-h IC50 of 0.08 mg/L based on a reduction in the biomass of algae. The study was conducted under static conditions and water concentrations were not measured. Partial water chemistry was reported. This study has been classified as secondary chronic toxicity information for an aquatic plant.

Calculation of the final uncertainty factor is shown on Table 3. A value of 105 was derived as the final uncertainty factor.

## 6.2 CALCULATION OF THE INTERIM PWQO VALUE

There is insufficient evidence to suggest that the aquatic toxicity of hexachlorocyclopentadiene is modified by water quality parameters such as hardness, pH or temperature. Therefore, the following Interim PWQO is set as a single value independent of other water quality parameters that might modify the toxicity.

The lowest observed toxic effect concentration considered valid for Interim PWQO development was a 30-day LC50 of 0.0067 mg/L for fathead minnow. This value has been divided by the final uncertainty factor of 105 to give a preliminary interim objective of 0.00006 mg/L or 0.06 µg/L (see Table 3). This preliminary interim objective is less than the odour protection value of 0.0005 mg/L. The odour protection value was calculated as half of the odour threshold concentration for hexachlorocyclopentadiene in water of 0.001 mg/L (Zoeteman *et al.* 1974 and WDNR 1989).

Therefore, the preliminary interim objective of 0.06 µg/l is recommended as the Interim Provincial Water Quality Objective for hexachlorocyclopentadiene.

## 7.0 RESEARCH NEEDS

A primary chronic toxicity study for a cold-water fish species, a study on one other fish species (either warm- or cold-water), and a study on a non-crustacean invertebrate are required for the development of a Provincial Water Quality Objective for hexachlorocyclopentadiene. At least one of these fish species must be resident in Ontario. Mutagenicity data obtained using aquatic test systems are also required. Additional aquatic toxicological information (e.g. acute and chronic toxicity studies) may be useful in reducing the uncertainty factor for the Interim PWQO for hexachlorocyclopentadiene. Minimum data requirements for

the development of a Provincial Water Quality Objective are described in greater detail in OMOE (1992a).

## 8.0 OBJECTIVES OF OTHER AGENCIES

In U.S. EPA's (1980) evaluation of hexachlorocyclopentadiene, no guideline was established since minimum data base requirements were not met. A hexachlorocyclopentadiene standard of 0.45 µg/L for fishing and fish propagation was set by New York State (NYSDEC 1987). New York State also set a value of 4.5 µg/L for fishing and fish survival. A non-drinking water aquatic chronic guideline of 0.5 µg/l for hexachlorocyclopentadiene has been set by the State of Michigan (MDNR 1988). No other hexachlorocyclopentadiene water guidelines for aquatic life were found (CCREM 1987; U.S. EPA 1988a, 1988b). Several drinking water guidelines have been set for hexachlorocyclopentadiene (OMOE 1992b). U.S. EPA's Ambient Drinking Water Criteria (for waters used as a source of drinking water and for fish consumption) is 206 µg/L, and both the Maximum Contaminants Level (lowest practical level) and a Maximum Contaminant Level Health Goal (a no health risk level) are set at 50 µg/L. New York State has an Ambient Water Quality Standard (for drinking water source protection) of 1 µg/L.



## 9.0 REFERENCES

- Applegate, V.C., J.H. Howell, A.E. Hall, Jr., and M.A. Smith. 1957. Toxicity of 4,346 Chemicals to Larval Lampreys and Fishes. Spec. Sci. Rep. Fish. No. 207, Fish Wild. Serv., U.S.D.I., Wash., D.C. 157 pp.
- Buccafusco, R.J. and G.A. LeBlanc. 1977. Acute toxicity of DNR 1989. Surface Water Quality Criteria for Toxic Substances. Hexachlorocyclopentadiene to bluegill (*Lepomis macrochirus*), channel catfish (*Ictalurus punctatus*), fathead minnow (*Pimephales promelas*) and the water flea (*Daphnia magna*). E.G. & G. Bionomics. Toxicity Test Report submitted to Velsicol Chemical Corporation, Chicago IL. (Cited in U.S. EPA 1980 and U.S. EPA 1984)
- Callahan, M., M. Slimak, N. Gabel, I. May, C. Fowler, R. Freed, P. Jennings, R. Durfee, F. Whitmore, B. Maestri, W. Mabey, B. Holt, and C. Gould. 1979. Water-Related Environmental Fate of 129 Priority Pollutants, Volume II. U.S. Environmental Protection Agency, Wash. D.C., EPA 440/4-79-029b.
- CCREM. 1987. Canadian Water Quality Guidelines. Task Force on Water Quality Guidelines of the Canadian Council of Resource and Environmental Ministers.
- Chou, S.F.J. and R.A. Griffin. 1983. Soil, clay, and caustic soda effects on solubility, sorption and mobility of hexachlorocyclopentadiene. Springfield, Virginia. National Technical Information Service. 54 pp. (PB84-116060) (Environmental Geology Notes No. 104). (Cited in WHO 1991)
- Chou, S.F.J., R.A. Griffin, M.M. Chou, and R.A. Larson. 1987. Products of hexachlorocyclopentadiene (C-56) in aqueous solution. Environ. Toxicol. Chem. 6:371-376.
- Davis, J.T. and W.S. Hardcastle. 1959. Biological assay of herbicides for fish toxicity. Weeds 7:397-404.
- Environment Canada. 1984. 1980-1981 Cornwall Industrial Survey. Draft. Pollution Control Division, Environmental Protection Service - Ontario Region, Toronto, Ontario.
- Freitag, D., H. Geyer, A. Kraus, R. Viswanathan, D. Kotzias, A. Attar, W. Klein, and F. Korte. 1982. Ecological profile analysis. VII. Screening chemicals for their environmental behaviour by comparative evaluation. Ecotoxicol. Environ. Safety 6:60-81.
- Geiger, D. 1987. Personal Communication. Unpublished data on hexachlorocyclopentadiene toxicity.

- Geyer, H., R. Viswanathan, D. Freitag and F. Korte. 1981. Relationship between water solubility of organic chemicals and their bioaccumulation by the alga chlorella. *Chemos.* 10:1307-1313.
- Graham, H. 1993. Personal Communication. Drinking Water Section, Water Resources Branch, Ontario Ministry of the Environment and Energy.
- Health and Welfare Canada. 1992. Guidelines for Canadian Recreational Water Quality. Ottawa, Ontario, Canada. 101 pp.
- Henderson, D. 1956. Bioassay investigations for International Joint Commission. Hooker Electrochemical Co., Niagara Falls, N.Y. U.S. Dept. Health, Educational and Welfare. Robert A. Taft Sanitary Engineering Center, Cincinnati, OH. (Cited in U.S. EPA 1980)
- Howard, P.H., R.S. Boethling, W.F. Jarvis, W.M. Meylan and E.M. Michalenko. 1991. Handbook of Environmental Degradation Rates. Lewis Publishers, Inc., Chelsea, Michigan.
- Kilzer, L., I. Scheunert, H. Geyer, W. Klein and F. Korte. 1979. Laboratory screening of the volatilization rates of organic chemicals from water and soils. *Chemosphere* 8:751-761. (Cited in WHO 1991)
- Kuhn, R. and M. Pattard, K. D. Pernak and A. Winter. 1989. Results of the harmful effects of water pollutants to *Daphnia magna* in the 21 day reproduction test. *Water Res.* 23(4):501-510.
- Kuhn, R. and M. Pattard. 1990. Results of the harmful effects of water pollutants to green algae (*Scenedesmus subspicatus*) in the Cell Multiplication Inhibition Test. *Water Res.* 24(1):31-38
- Leo, A. and D. Weininger. 1988. Daylight Software Version 3.53 for Vax -11 under VMS 4.6+, CLOGP version 3.4. Pomona Medicinal Chemistry Project, Pomona College, Claremont, C.A. Distributed by Daylight Chemical Information Systems, Inc., 3951 Claremont St., Irvine C.A. 92714. (Cited in U.S. EPA 1993)
- Lu, P.Y., R.L. Metcalf, A.S. Hirwe and J.W. Williams. 1975. Evaluation of environmental distribution and fate of hexachlorocyclopentadiene, chlordene, heptachlor, and heptachlor epoxide in a laboratory model ecosystems. *J. Agric. Food Chem.* 23(5):967-973.
- Mackay, D. 1982. Correlation of bioconcentration factors. *Environ. Sci. Technol.* 16:274-278.

- MacPhee, C, and R. Ruelle. 1969. Lethal Effects of 1888 Chemicals Upon Four Species of Fish From Western North America. University of Idaho. Forest, Wild. Range Exp. Station Bull. No. 3, Moscow, ID, 112 p.
- MDNR 1988. Rule 57(2) Guideline Levels. Letter from P. D. Zugger, Surface Water Quality Division. State of Michigan. 2 pp.
- Meirer, J.R., H.P. Ringhand, W.E. Coleman, J.W. Munch, R.P. Streicher, W.H. Kaylor, and K.M. Schenck. 1985. Identification of mutagenic compounds formed during the chlorination of humic acid. *Mutat. Res.*, 157: 111-122. (Cited in WHO 1991)
- Naishstein, S.Y. and E.V. Lisovskaya. 1965. Maximum permissible concentration of hexachlorocyclopentadiene in water bodies. *Gigiena i Sanitariya (Trans.) Hyg. Sanit.* 30: 177. (Cited in U.S. EPA 1980)
- National Research Council. 1978. Kepone/Mirex/Hexachlorocyclopentadiene: An environmental assessment. Scientific and technical assessments of environmental pollutants. Environmental Studies Board, Commission on Natural resources, National Research Council. National Academy of Science, Washington, D.C. 73 p.
- NYSDEC. 1987. New York State Ambient Water Quality Standards and Guidance Values New York State Department of Environmental Conservation, Albany, New York. 37 p.
- Oliver, B.G. and A.J. Niimi. 1985. Bioconcentration factors of some halogenated organics for rainbow trout: limitations in their use for prediction of environmental residues. *Environ. Sci. Technol.* 19:842-849.
- OMOE. 1987. The Effluent Monitoring Priority Pollutants List (1987). Hazardous Contaminants Coordination Branch, Ontario Ministry of the Environment. 66 p. & append.
- OMOE. 1988. Thirty Seven Municipal Water Pollution Control Plants - Pilot Monitoring Study. Volume 1 - Interim Report. Water Resources Branch, Ontario Ministry of the Environment. 97 p.
- OMOE. 1991. Preliminary report for the first six months of monitoring in the pulp and paper sector (January 1, 1990 to June 30, 1990). Municipal-Industrial Strategy for Abatement. Water Resources Branch, Ontario Ministry of the Environment. 175 p.
- OMOE. 1992a. Ontario's water quality objective development process. Aquatic Criteria Development Committee, Ontario Ministry of the Environment. 50 p.
- OMOE. 1992b. Parameters Listing System (PALIS). Ontario Ministry of the Environment. 51 p.

- OMOE. 1993. Twelve Month Data Report: Organic Chemical Manufacturing Sector (October 1, 1989 to September 30, 1990). Municipal-Industrial Strategy for Abatement. Water Resources Branch, Ontario Ministry of the Environment. 38 p. (unpublished).
- Podowski, A.A. and M.A.Q. Khan. 1984. Fate of hexachlorocyclopentadiene in water and goldfish. Arch. Environ. Contam. Toxicol. 13:471-481.
- Podowski, A.A. S.L. Sclove, A. Pilipowicz, and M.A.Q. Khan. 1991. Biotransformation and disposition of hexachlorocyclopentadiene in fish. Arch. Environ. Contam. Toxicol. 20:488-496.
- Sinhaseni, P., L.G. D'Alecy, R. Hartung, and M. Schlafer. 1983. Respiratory effects of hexachlorocyclopentadiene on intact rainbow trout (*Salmo gairdneri*) and on oxidative phosphorylation of isolated trout heart mitochondria. Toxicol. Appl. Pharmacol. 67:215-223.
- Spehar, R.L., G.D. Veith, D.L. Defoe, and B.V. Bergstedt. 1979. Toxicity and bioaccumulation of hexachlorocyclopentadiene, hexachloronobornadiene and heptachloronobornene in larval and early juvenile fathead minnows, *Pimephales promelas*. Bull. Environ. Contam. Toxicol. 21:576-583.
- Staples, C.A., A.F. Werner, and T.J. Hoogheem. 1985. Assessment of priority pollutant concentrations in the United States using STORET database. Environ. Toxicol. Chem. 4:131-142.
- U.S. EPA. 1977. A Rapid Assessment of the Toxicity of Three Chlorinated Cyclodiene Insecticide Intermediates to Fathead Minnows. Environmental Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency. Duluth, Minnesota. EPA-600/3-77-099.
- U.S. EPA. 1980. Ambient Water Quality Criteria for Hexachlorocyclopentadiene. Office of Water Regulations and Standards, Criteria and Standards Division, U.S. Environmental Protection Agency, Wash., D.C. EPA 440/5-80-055.
- U.S. EPA. 1984. Health Assessment Document for Hexachlorocyclopentadiene. Office of Research and Development, Office of Health and Environmental Assessment, Environmental Criteria and Assessment Office, U.S. Environmental Protection Agency, Cincinnati, Ohio. EPA-600/8-84-001F
- U.S. EPA. 1988a. Water Quality Standards Criteria Summaries: A Compilation of State/Federal Criteria: Organics. U.S. Environmental Protection Agency, Wash., D.C. NTIS PB89-141386.



- U.S. EPA. 1988b. State Water Quality Standards Summaries. U.S. Environmental Protection Agency, Wash., D.C. NTIS PB89-141634.
- U.S. EPA. 1993. ASTER Ecotoxicity Profile. U.S. Environmental Protection Agency, Environmental Research Laboratory - Duluth.
- Veith, G.D., D.L. Defoe, and B.V. Bergstedt. 1979. Measuring and estimating the bioconcentration factor of chemicals in fish. J. Fish. Res. Board Can. 36:1040-1048.
- Vilkas, A.G. 1977. The acute toxicity of hexachlorocyclopentadiene to the water flea (*Daphnia magna*). Union Carbide Environmental Services. Prepared for Velsicol Chemical Corporation, Chicago, IL. (Cited in U.S. EPA 1980 and U.S. EPA 1984).
- WDNR 1989. Chapter NR 102. Water quality standards for Wisconsin surface waters. Wisconsin Department of Natural Resources. Register No. 398.
- Weast, R.C. 1988-89. CRC Handbook of data on organic compounds. CRC Press. Boca Raton, FL.
- Wolfe, N.L., R.G. Zepp, P. Schlotzhauer, and M. Sink. 1982. Transformation pathways of hexachlorocyclopentadiene in the aquatic environment. Chemos. 11:91-101.
- World Health Organization. 1991. Hexachlorocyclopentadiene. Environmental Health Criteria 120. Geneva.
- Yu, C.C. and Y.H. Atallah. 1977. HEX hydrolysis at various pHs and temperatures. Chicago, Velsicol Chemical Corporation (Project No. 482428, Report No. 8 - Laboratory Report). (Cited in WHO 1991)
- Zepp, R.G., N.L. Wolfe, G.L. Baughman, P.F. Schlotzhauer and J.N. MacAllister. 1979. Dynamics of processes influencing the behaviour of hexachlorocyclopentadiene in the aquatic environment. U.S. Environmental Protection Agency (ERL), Athens, Ga. (Paper presented before the Division of Environmental Chemistry, American Chemical Society, Washington, D.C. September 9-14, 1979). (Cited in Callahan *et al.* 1979).
- Zoeteman, B.C.J., G.J. Piet, C.T.M. Ruygrok and R. Van de Heuvel. 1974. Threshold Odour Concentrations in Water of Chemical Substance. Annex to Bulletin No. 73-7, National Institute for Water Supply. The Hague, the Netherlands. (Cited in Lillard *et al.* 1975)



## APPENDICES





**TABLE 1: PHYSICAL-CHEMICAL PROPERTIES**

<b>COMPOUND:</b>	<b>CHEMICAL FORMULA:</b>	<b>CAS No.:</b>
hexachlorocyclopentadiene	C <sub>5</sub> Cl <sub>6</sub>	77-47-4

**PROPERTIES**

MOLECULAR WEIGHT (MW):	272.77 (CRC Index 1990/91)
MELTING POINT:	-9 °C (CRC Index 1990/91)
BOILING POINT:	239 °C (CRC Index 1990/91)
PHYSICAL STATE AT ROOM TEMP.:	dense liquid (WHO 1991)
DISSOCIATION CONSTANT:	
LIQUID DENSITY (D):	1.7019 @ 25°C/4°C (CRC Index 1990/91)
MOLAR VOLUME (MW/D):	160.3 cm <sup>3</sup> /mol (calculated)
VAPOUR PRESSURE (Ps):	10.7 Pa (Wolfe <i>et al.</i> 1982)
WATER SOLUBILITY (Cs):	1.8 mg/L (Wolfe <i>et al.</i> 1982)
HENRY'S LAW (Ps/Cs):	2.7 X 10 <sup>-2</sup> atm m <sup>3</sup> /mole (Wolfe <i>et al.</i> 1982)

**PERSISTENCE**

B.O.D.:	
BREAKDOWN PRODUCTS:	hexachloro-2-cyclopentenone; hexachloro-3-cyclopentenone
HALF-LIFE (DAYS):	half-life > 20 days, most >100 days (USEPA 1993)

**OCTANOL-WATER PARTITION COEFFICIENT (K<sub>ow</sub>)**

RANGE OF AVAILABLE Log K <sub>ow</sub> VALUES:	3.99 to 5.51
FINAL CHOSEN Log K <sub>ow</sub> VALUE:	4.6 (Leo and Weininger 1988)

**BASELINE UNCERTAINTY FACTOR FOR GUIDELINE DEVELOPMENT**

IF valid BCF < 1000, USE 1000	
IF valid BCF ≥ 10,000, USE 10000	
BASELINE UNCERTAINTY FACTOR:	<div style="border: 1px solid black; padding: 2px 10px; display: inline-block;">1000</div> ENTER THIS VALUE ON TABLE 3



TABLE 2: AQUATIC TOXICITY DATA TABLE FOR HEXACHLOROCYCLOPENTADIENE

SPECIES	LIFE STAGE	RESPONSE	TEST CONDITIONS					EFFECT CONC. (mg/L)	DATA CODES <sup>1</sup>	REFERENCE
			pH	TEMP. (°C)	DO (mg/L)	ALK. (mg/l)	HARD. (mg/L)			
VERTEBRATES										
Primary Data										
fathead minnow ( <i>Pimephales promelas</i> )	larval + early juvenile (one-day- old)	96-h LC50 30-d LC50 30-d NOEC	7.2-7.7	25±2	7.2-8.6	42-43	45-47	0.0070 0.0067 0.0037	A,F,M C,F,M C,F,M	Spehar <i>et al.</i> 1979
Secondary Data										
fathead minnow	juvenile (0.06 g)	96-h EC50 96-h LC50	7.2	21.5	7.8	44	48	0.030 0.030	A,S,M	Geiger, unpublished data, 1987
fathead minnow		96-h LC50 96-h LC50 (using acetone) 96-h LC50 (using emulsion)	7.4 8.2 8.2				40 400 400	0.104 0.078 0.059	A,S,U	Henderson 1956
fathead minnow	0.72 g	24-h LC50 48-h LC50 96-h LC50 NOEC		22			soft	0.240 0.210 0.180 0.087	A,S,U	Buccafusco and LeBlanc 1977 (cited in U.S. EPA 1984)
bluegill sunfish ( <i>Lepomis macrochirus</i> )	fingerling (3-5 in.)	24-h LC50 48-h LC50 96-h LC50	6.6-7.4	25±1	7.1-7.7		25-30	>500 30 25	A,S,U	Davis and Hardcastle 1959

<sup>1</sup> DATA CODE KEY

A = acute  
S = static  
U = unmeasured nominal conc.  
? = unknown

C = chronic  
R = static/renewal  
F = flow-through  
M = measured conc.

QSAR = Quantitative Structure-Activity Relationships



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SPECIES	LIFE STAGE	RESPONSE	TEST CONDITIONS					EFFECT CONC. (mg/L)	DATA CODES <sup>1</sup>	REFERENCE
			pH	TEMP. (°C)	DO (mg/L)	ALK. (mg/l)	HARD. (mg/L)			
bluegill sunfish	0.45 g	24-h LC50 48-h LC50 96-h LC50 NOEC		22			soft	0.170 0.150 0.130 0.065	A,S,U	Buccafusco and LeBlanc (cited in U.S. EPA 1984)
bluegill sunfish	fingering	mort., 15 min. mort., 30 min. mort., 30 min. no effect, 24 h	7.5-8.2	14	8.6-13.7			5 5 1 0.1	A,S,U	Applegate <i>et al.</i> 1957
largemouth bass ( <i>Micropterus salmoides</i> )	fingering (3-5 in.)	24-h LC50 48-h LC50 96-h LC50	6.6-7.4	25±1	7.1-7.7		25-30	>500 35 20	A,S,U	Davis and Hardcastle 1959
rainbow trout ( <i>Oncorhynchus mykiss</i> )	268 g	mortality, 6.5 h		12				0.13	A,F,U	Sinhaseni <i>et al.</i> 1983
rainbow trout	fingering	mort., 15 min. mort., 30 min. mort., 1 h no effect, 24 h	7.5-8.2	14	8.6-13.7			5 5 1 0.1	A,S,U	Applegate <i>et al.</i> 1957
channel catfish ( <i>Ictalurus punctatus</i> )	2.1 g	24-h LC50 48-h LC50 96-h LC50 NOEC		22			soft	0.190 0.150 0.097 0.056	A,S,U	Buccafusco and LeBlanc (cited in U.S. EPA 1984)
chinook salmon ( <i>Oncorhynchus tshawytscha</i> )		mortality, 3 h	7.2	10		7	0-17	10	A,S,U	MacPhee and Ruelle 1969

<sup>1</sup> DATA CODE KEY

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**TABLE 2: AQUATIC TOXICITY DATA TABLE FOR HEXACHLOROCYCLOPENTADIENE**

SPECIES	LIFE STAGE	RESPONSE	TEST CONDITIONS					EFFECT CONC. (mg/L)	DATA CODES <sup>1</sup>	REFERENCE
			pH	TEMP. (°C)	DO (mg/L)	ALK. (mg/l)	HARD. (mg/L)			
coho salmon ( <i>Onchorhynchus kisutch</i> )		mortality, 3 h	7.2	10		7	0-17	10	A,S,U	MacPhee and Ruelle 1969
northern squawfish ( <i>Ptychocheilus oregonensis</i> )		mortality, 3 h	7.2	10		7	0-17	10	A,S,U	MacPhee and Ruelle 1969
sea lamprey ( <i>Petromyzon marinus</i> )	juvenile	mortality, 11 h mortality, 1 h mort., 30 min. no effect, 24 h	7.5-8.2	14	8.6-13.7			5 5 1 0.1	A,S,U	Applegate <i>et al.</i> 1957
goldfish ( <i>Carassius auratus</i> )	1.0 to 2.95 g	LT50s 9.1 to 16.6 h		21-22				0.18	A,S,U	Podowski <i>et al.</i> 1991
<b><u>INVERTEBRATES</u></b>										
<b><i>Primary Data</i></b>										
<i>Daphnia magna</i>	24 h-old	24-h EC50 21-d LOEC (parent animal mortality) 21-d NOEC	8±0.2	25±1	>58% sat.			0.21 0.019  0.009	A,S,U C,R,M  C,R,M	Kuhn <i>et al.</i> 1989
<b><i>Secondary Data</i></b>										
<i>Daphnia magna</i>		24-h LC50 48-h LC50 NOEC		22			soft	0.130 0.039 0.018	A,S,U	Buccafusco and LeBlanc (cited in U.S. EPA 1984)

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TABLE 2: AQUATIC TOXICITY DATA TABLE FOR HEXACHLOROCYCLOPENTADIENE

SPECIES	LIFE STAGE	RESPONSE	TEST CONDITIONS					EFFECT CONC. (mg/L)	DATA CODES <sup>1</sup>	REFERENCE
			pH	TEMP. (°C)	DO (mg/L)	ALK. (mg/l)	HARD. (mg/L)			
<i>Daphnia magna</i>		24-h LC50 48-h LC50 NOEC		17			soft	0.093 0.052 0.032	A,S,U	Vilkas 1977 (cited in U.S. EPA 1984)
mosquito ( <i>Culex pipiens quinquefasciatus</i> )	larvae	LC50						2.3	A,?,?	Lu <i>et al.</i> 1975
<b>PLANTS</b>										
<b>Secondary Data</b>										
algae ( <i>Scenedesmus subspicatus</i> )	3-d old test culture	48-h IC50 (biomass) 48-h IC50 (growth)	8.1-9.6	24±1				0.08 0.24	C,S,U	Kuhn and Pattard 1990

<sup>1</sup> DATA CODE KEY

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S = static      R = static/renewal      F = flow-through  
U = unmeasured nominal conc.      M = measured conc.  
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# Table 3: UNCERTAINTY FACTOR WORKSHEET

CHEMICAL:

HEXACHLOROCYCLOPENTADIENE

CAS No.:

77-47-4

CONCENTRATION UNITS:

mg/L

Test Conditions		Species (life stage)	Toxicity End-point	Effect Conc.	Data Codes	Data Type	Calibration Factor	Reference
ACUTE	VERTEBRATE	fathead minnow (juvenile)	96-h LC50	0.007	F,M	1°	0.8	Spehar <i>et al.</i> 1979
		channel catfish	96-h LC50	0.097	S,U	2°	0.9	Buccafusco and LeBlanc (1977)
		rainbow trout	mortality, 6.5 h	0.13	F,U	2°	0.9	Sinhaseni <i>et al.</i> 1983
	INVERT	<i>Daphnia magna</i> (24 h-old)	24-h EC50	0.21	S,U	2°	0.9	Kuhn <i>et al.</i> 1989
CHRONIC	VERTEBRATE	fathead minnow (juvenile)	30-d LC50	0.0067	F,M	1°	0.5	Spehar <i>et al.</i> 1979
		bluegill	simulated 30-d LC50	0.12	S,U	3°	0.8	ACR: Spehar <i>et al.</i> 1979; Endpoint: Buccafusco and LeBlanc (1977)
	INVERT	<i>Daphnia magna</i> (24 h-old)	21-d LOEC	0.019	R,M	1°	0.5	Kuhn <i>et al.</i> 1989
	PLANT	algae	48-h IC50 (biomass)	0.08	S,U	2°	0.9	Kuhn and Pattard 1990

## CALCULATION OF FINAL UNCERTAINTY FACTOR:

Since the BCF < 1000, the baseline uncertainty factor = 1000

Baseline Uncertainty Factor X Calibration Factors (maximum number = 11)

1000 x 0.8 x 0.9 x 0.9 x 0.9 x 0.5 x 0.8 x 0.5 x 0.9 x  x  x

105

FINAL UNCERTAINTY FACTOR

CRITICAL VALUE + FINAL UNCERTAINTY FACTOR PWQG VALUE

= 0.0067 + 105 = 0.00006 mg/L

Assign 2 DATA CODES, one from each of the following rows:

S = static R = static/renewal F = flow-through

U = unmeasured nominal conc. M = measured conc.

DATA TYPE:

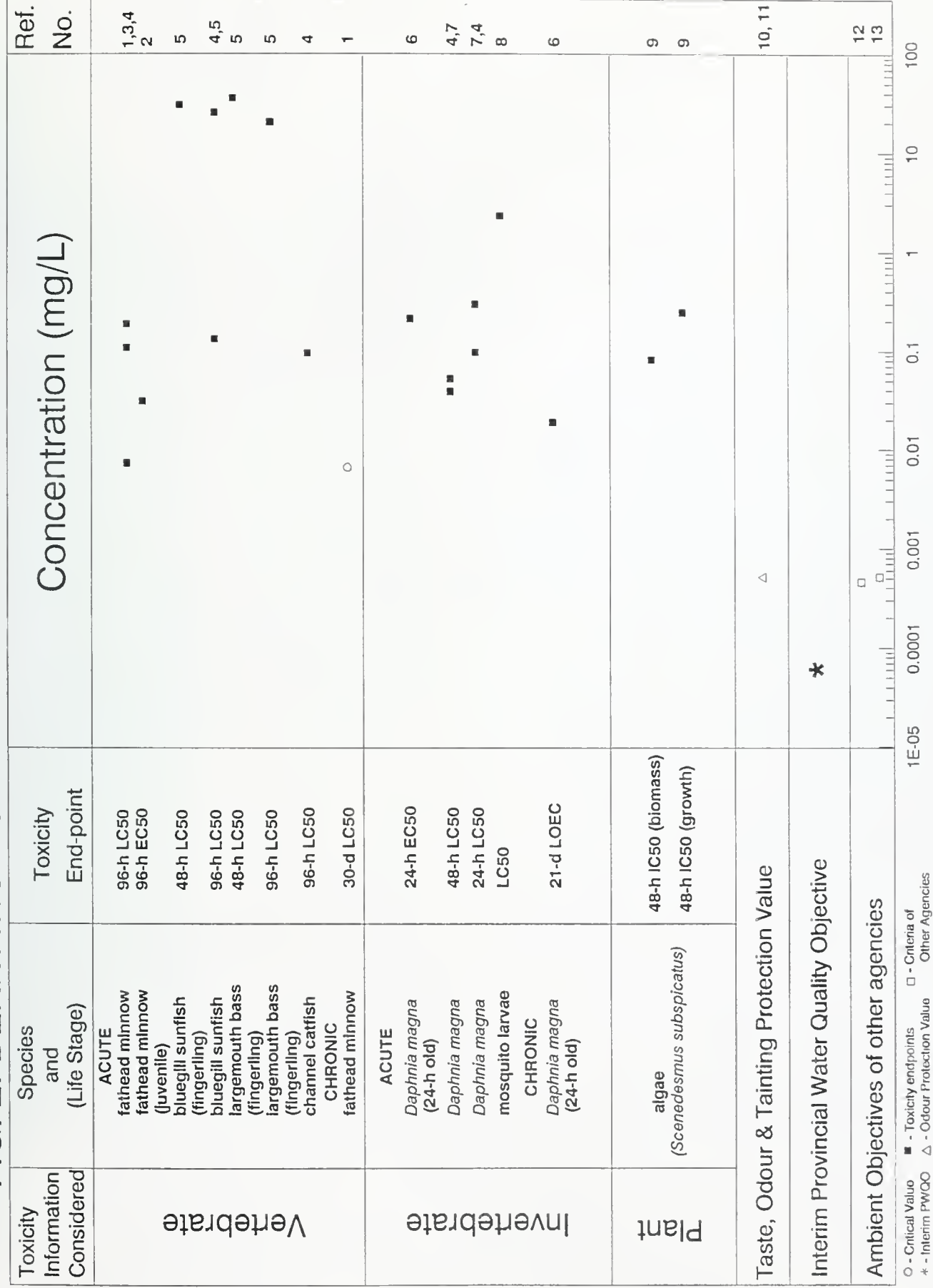
1° = Primary 2° = Secondary 3° = Simulated Data

? = Unknown (Default Data Quality = 2°)





FIG. 2: DERIVATION GRAPH - HEXACHLOROCYCLOPENTADIENE





## Key to References for Figure 2

<u>Figure 2 Reference Number</u>	<u>Reference</u>
1	Spehar <i>et al.</i> (1979)
2	Geiger (1987, unpublished data)
3	Henderson (1956)
4	Buccafusco and LeBlanc (1977)
5	Davis and Hardcastle (1959)
6	Kuhn <i>et al.</i> (1989)
7	Vilkas (1977)
8	Lu <i>et al.</i> (1975)
9	Kuhn and Pattard (1990)
10	Zoeteman <i>et al.</i> (1974)
11	WDNR (1989)
12	NYSDEC (1987)
13	MDNR (1988)





